

## Supplementary information for

### Unprecedented coexistence of cyano-bridged $\text{Mn}_4^{\text{III}}\text{Cr}^{\text{III}}$ and $\text{Mn}_2^{\text{III}}\text{Cr}^{\text{III}}$ heterobimetallic complexes in one single crystal

Diana Visinescu, Luminita Marilena Toma, Francesc Lloret, Oscar Fabelo, Catalina Ruiz-Pérez and Miguel Julve

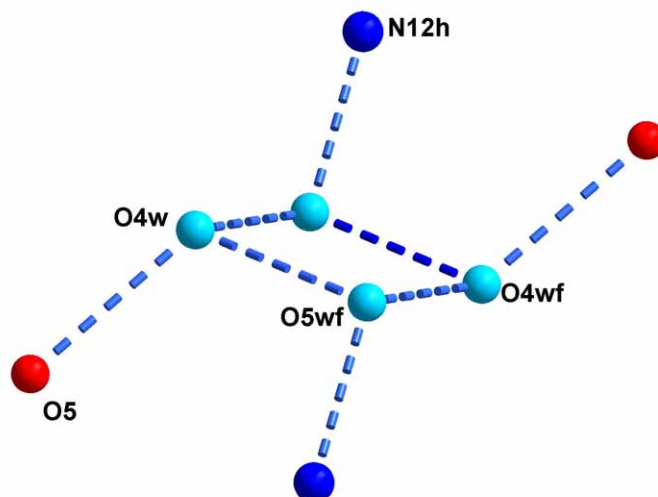
**Table S1.** Hydrogen bond distances (Å) and angles (°) in compound **1**.

D-H...A	O-H (Å)	H...O (Å)	D...A (Å)	< D-H...A (°)
O1W-H11W...N11	0.74(5)	2.13(6)	2.827(5)	156(6)
O1W-H12W...O1c	0.77(5)	2.08(5)	2.849(4)	172(5)
O2W-H21W...O7d	0.68(10)	2.34(9)	2.898(6)	140(9)
O2W-H22W...O6d	0.92(9)	1.93(9)	2.800(5)	158(9)
O3W-H31W...O12e	0.71(5)	2.28(6)	2.952(5)	158(6)
O3W-H32W...N4e	0.68(6)	2.18(6)	2.838(6)	164(6)

D...A (Å)		D...A	
O4W...O5W	2.784(2)	O4W...O5g	3.011(2)
O5W...O4Wf	2.945(2)	O5W...N12h	2.856(2)

Symmetry code: (c)  $2 - x, -y, -z$ ; (d)  $2-x, 1-y, 1-z$ ; (e)  $1-x, -y, 1-z$ ; (f)  $1-x, 1-y, -z$ ;  
(g)  $-1+x, y, z$ ; (h)  $x, 1+y, z$

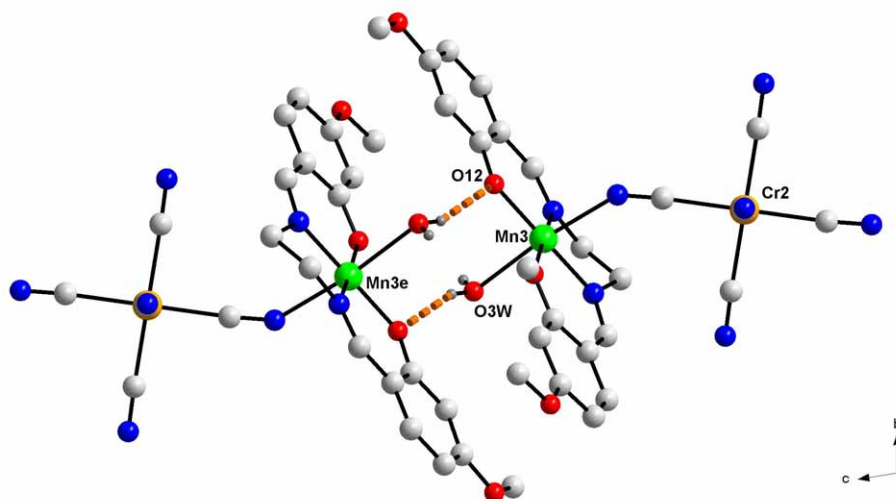


**Fig. S1.** View of the cyclic quasi-planar tetramer builded by lattice water molecules

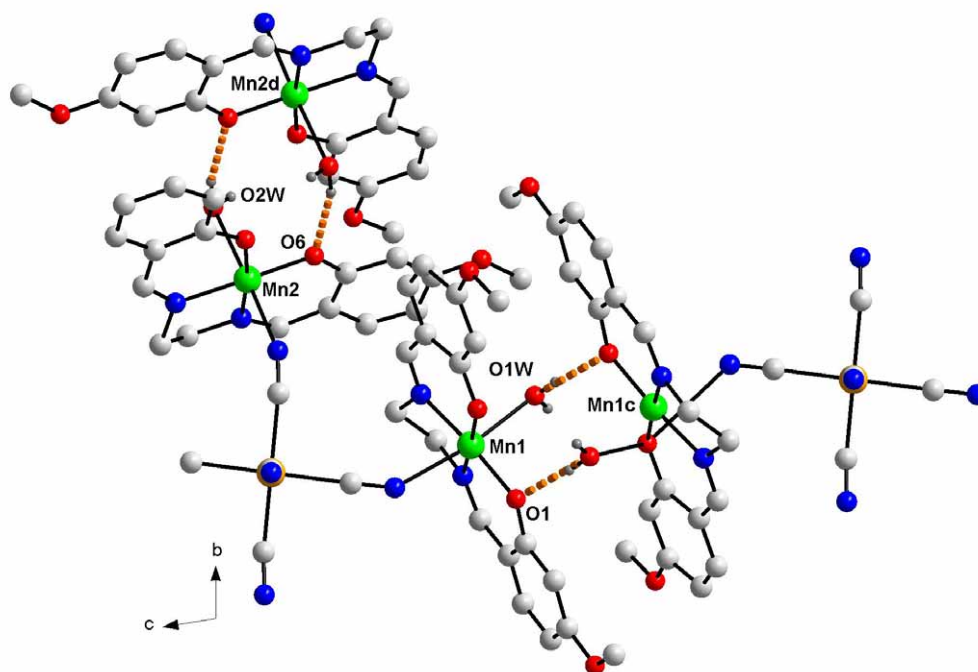
**Table S2.** Intermetallic distances (Å)

Pentameric unit		Trimeric units		
	<b>Intramolecular</b>			
Cr1...Mn1a	5.2255(5)	Cr2...Mn3b	5.2121(5)	
Cr1...Mn2a	5.2813(3)			
	<b>Intermolecular</b>			
Mn1...Mn1c	5.0332(4)	Mn3...Mn3e	5.2530(5)	
Mn2...Mn2d	4.9144(3)			

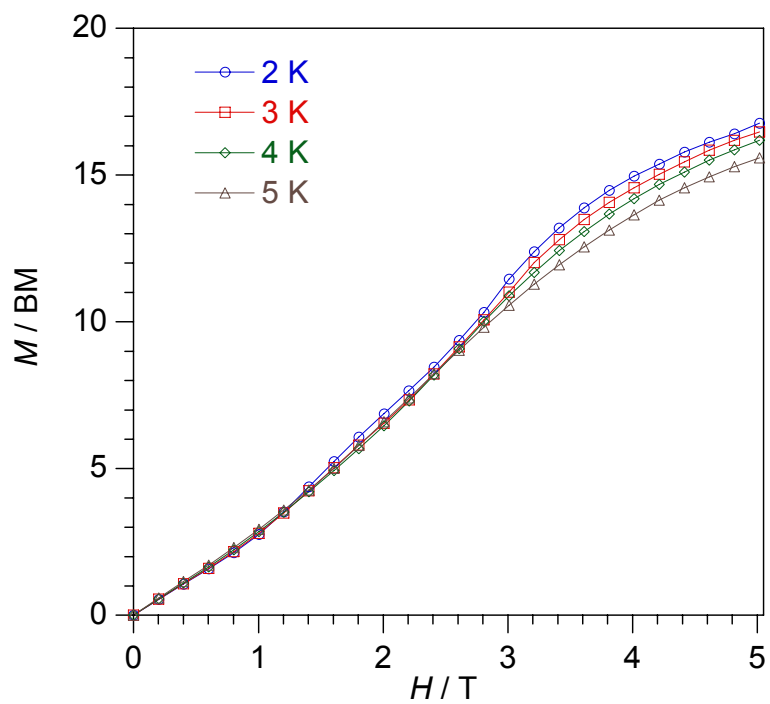
Symmetry code: (a) 2-x, -y, 1-z; (b) 1-x, -y, -z; (c) 2-x, -y, -z; (d) 2-x, 1-y, 1-z; (e) 1-x, -y, 1-z



**Figure S2.** Hydrogen-bonds in the pentanuclear unit of **1**



**Figure S3.** Hydrogen-bonds in the trinuclear unit of **1**



**Fig. S4.** Magnetization vs.  $H$  plot of **1** at 2.0-5.0 K.